Structural Characterization of Molybdnumniobate Clusters

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Introduction: Framework structures in which the tenants are transition elements, represents a growing area of novel molecular sieves. In an attempt to synthesize molybdnumniobate framework material by hydrothermal methods, single crystals of a novel material consisting of molybdnumniobate clusters, charge balanced by hydrogen-bonded tripropylamine (TPA) and water were obtained. The synchrotron X-ray diffraction studies revealed that the compound crystallizes in the orthorhombic space group ***Pccn,*** with cell dimensions *a* = 21.240(3), *b* = 21.830(4), *c* = 16.739(3) Å, V = 7761(3) Å^3, *R* = 0.0475, R_w = 0.14659 [6943 observed reflections with I > 2σ]. Each cluster consists of three Nb octahedra and four Mo tetrahedra. Two Nb octahedra share an edge and one of the corners of this shared edge is connected to a Mo tetrahedron, which is corner connected to the third Nb octahedron. The second Mo tetrahedron shares two of its corners with the apices of edge sharing Nb octahedra and the third corner with the third Nb octahedron. Finally two more Mo tetrahedra are corner linked to this edge sharing Nb unit, with one of them sharing a corner with the third Nb octahedra. These clusters are held together by charge compensating TPA, organic amines and water molecules through weak hydrogen bonds (**Figure 1**).

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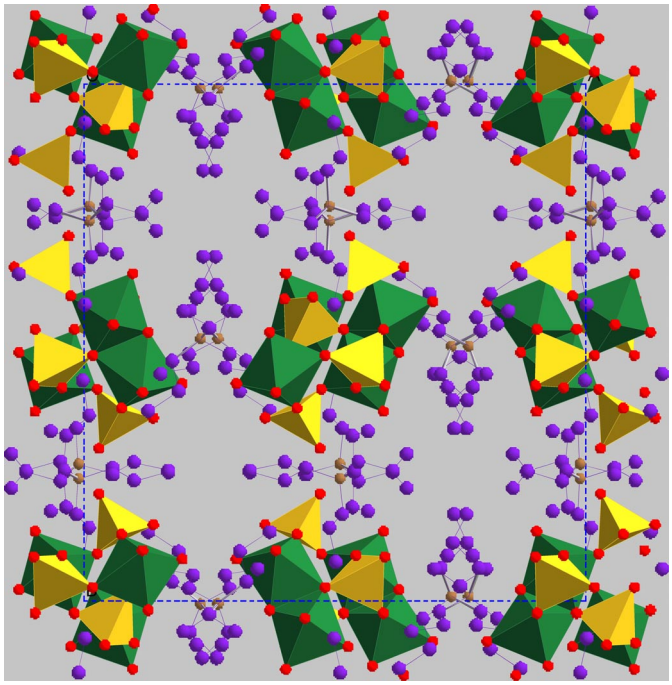

Figure 1. A polyhedral and ball and stick representation of the structure of a molybdnumniobate cluster. The green octehedra representing Nb sites are corner connected to yellow Mo tetrahedra. The clusters are hydrogen bonded to charge compensating TPA units shown in purple (C sites) and brown (N sites). Water molecules are shown for clarity.